



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:10 AM GMT

PDB ID : 3DLB
Title : Crystal structure of the guide-strand-containing Argonaute protein silencing complex
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Deposited on : 2008-06-26
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

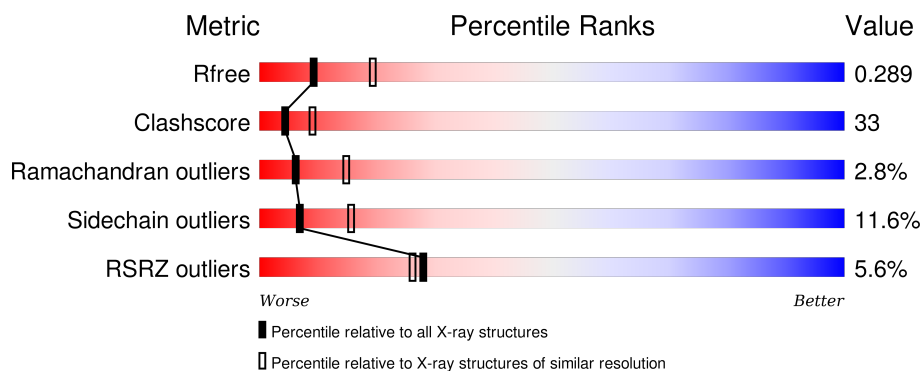
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	685	<div> <div>4%</div> <div>51%</div> <div>34%</div> <div>7%</div> <div>7%</div> </div>
1	B	685	<div> <div>7%</div> <div>45%</div> <div>37%</div> <div>7%</div> <div>10%</div> </div>
2	X	10	<div> <div>20%</div> <div>30%</div> <div>50%</div> </div>
2	Y	10	<div> <div>40%</div> <div>10%</div> <div>50%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9793 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	9	0	0
			4891	3125	913	846	7			
1	B	614	Total	C	N	O	S	34	0	0
			4668	2983	873	806	6			

- Molecule 2 is a DNA chain called DNA (5'-D(*DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	5	Total	C	N	O	P	0	0	0
			101	50	19	28	4			
2	Y	5	Total	C	N	O	P	0	0	1
			85	40	17	24	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	19	Total	O	0	0
			19	19		
3	X	3	Total	O	0	0
			3	3		
3	Y	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.85Å 123.40Å 84.91Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 32.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.70) 94.2 (32.82-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.293 0.254 , 0.289	Depositor DCC
R_{free} test set	2153 reflections (5.48%)	DCC
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42792 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9793	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	3/5009 (0.1%)	0.86	12/6817 (0.2%)
1	B	0.52	4/4780 (0.1%)	0.86	14/6509 (0.2%)
2	X	0.93	0/113	1.19	0/173
2	Y	0.55	0/95	0.95	0/146
All	All	0.57	7/9997 (0.1%)	0.86	26/13645 (0.2%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	TRP	CB-CG	-13.53	1.25	1.50
1	A	503	TRP	CB-CG	-11.07	1.30	1.50
1	A	415	TRP	CB-CG	-5.93	1.39	1.50
1	B	640	ARG	CB-CG	-5.35	1.38	1.52
1	B	387	GLN	CB-CG	-5.31	1.38	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	LEU	N-CA-C	10.63	139.69	111.00
1	A	608	ARG	N-CA-C	-9.09	86.45	111.00
1	A	609	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	356	GLY	N-CA-C	7.85	132.73	113.10
1	B	102	ASP	CB-CG-OD1	-7.66	111.41	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4891	0	4892	292	0
1	B	4668	0	4624	345	0
2	X	101	0	59	7	0
2	Y	85	0	46	1	0
3	A	25	0	0	0	0
3	B	19	0	0	0	0
3	X	3	0	0	0	0
3	Y	1	0	0	0	0
All	All	9793	0	9621	632	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

The worst 5 of 632 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:PRO:HD3	1:B:522:LEU:HD21	1.28	1.12
1:A:175:CYS:HB2	1:A:265:LEU:HD11	1.28	1.08
1:B:237:GLU:HG3	1:B:237:GLU:O	1.51	1.08
1:B:349:LEU:HB2	1:B:381:LEU:HD12	1.38	1.05
1:B:440:ARG:HD3	1:B:441:GLU:N	1.71	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	633/685 (92%)	554 (88%)	61 (10%)	18 (3%)	6	15
1	B	604/685 (88%)	530 (88%)	57 (9%)	17 (3%)	6	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1237/1370 (90%)	1084 (88%)	118 (10%)	35 (3%)	6	15

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	SER
1	A	507	GLU
1	A	606	VAL
1	A	607	HIS
1	A	608	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	475/549 (86%)	424 (89%)	51 (11%)	8	19
1	B	447/549 (81%)	391 (88%)	56 (12%)	6	13
All	All	922/1098 (84%)	815 (88%)	107 (12%)	7	16

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	610	PHE
1	B	120	ARG
1	B	502	LEU
1	A	631	LEU
1	B	57	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	585	GLN
1	A	621	HIS
1	B	382	HIS

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Mol	Chain	Res	Type
1	A	516	GLN
1	B	419	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	637/685 (92%)	0.26	25 (3%) 43 43	43, 74, 102, 115	3 (0%)
1	B	614/685 (89%)	0.37	45 (7%) 18 16	46, 78, 116, 126	14 (2%)
2	X	5/10 (50%)	-0.10	0 100 100	57, 68, 87, 117	0
2	Y	5/10 (50%)	-0.30	0 100 100	68, 72, 76, 93	0
All	All	1261/1390 (90%)	0.31	70 (5%) 28 26	43, 76, 112, 126	17 (1%)

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	177	MET	5.6
1	A	607	HIS	5.0
1	A	437	VAL	4.8
1	B	143	PRO	4.4
1	B	144	GLY	4.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.